

```
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6 7 9 10
ring nodes :
1 2 3 4 5 16
chain bonds :
1-7 5-6 6-9 7-10
ring bonds :
1-2 1-5 1-16 2-3 2-16 3-4 3-16 4-5 4-16 5-16
exact/norm bonds :
1-2 1-5 1-16 2-3 2-16 3-4 3-16 4-5 4-16 5-16 6-9 7-10
exact bonds :
1-7 5-6
G1:P, As, Sb
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 9:CLASS 10:CLASS
16:Atom
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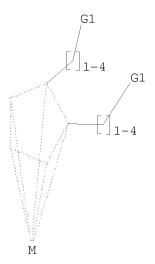
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L1

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L1 HAS NO ANSWERS

L1STR



G1 P, As, Sb

Structure attributes must be viewed using STN Express query preparation.

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32.0% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 120260 TO 129740 PROJECTED ANSWERS: 1 TO 168

L2. 1 SEA SSS SAM L1

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=> fil caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY

SESSION

1 ANSWERS

80 ANSWERS

FULL ESTIMATED COST 178.36 178.57

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=> s 13 L4

4 10 L3

=> d 1-10 bib abs

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:1204473 CAPLUS

DN 147:479320

TI Preparation of Group VIII metal phosphine complexes for use in the carbonylation of ethylenically unsaturated compounds

IN Eastham, Graham Ronald; Tindale, Neil

PA Lucite International UK Limited, UK

SO PCT Int. Appl., 153pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

FAN.	PATENT NO.					KIN	D	DATE		APPLICATION NO.						DATE			
ΡI	WO	2007119079			A1		20071025		WO 2007-GB50189						20070410				
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	CA,	
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DDAT	CD	2006	7.40	4		70		2006	0.412										

PRAI GB 2006-7494 A 20060413

OS CASREACT 147:479320; MARPAT 147:479320

AB The invention concerns metal complexes and their preparation, in particular a metal complex MLnXm, where M is a metal of Group 8, 9 or 10 and X is a halide, HCO3-, NO3-, CO32- or carboxylate, n is ≤ the coordination number of the metal, and m is 1 or 2 and is the oxidation state of the metal. The ligand L may be a phosphine, including a bidentate phosphine as defined buy a variety of formulas and specifically named compds. The

process of the complex production comprises reacting an ammine compound of metal

M with a complexing compound, which is preferably a phosphine. The complexes are claimed as catalysts for carbonylating an ethylenically unsatd. compound Advantages of the claimed complexes include: provides a stable catalyst metal complex without build-up of heavies during the catalytic process which would need periodic removal, no air sensitivity, and reduced catalyst preparation time.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
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- AN 2007:197719 CAPLUS
- DN 146:254034
- TI Improved carbonylation catalyst system
- IN Eastham, Graham Ronald; Tindale, Neil
- PA Lucite International UK Limited, UK
- SO PCT Int. Appl., 111pp. CODEN: PIXXD2
- DT Patent
- LA English
- FAN.CNT 1

r An.	_	TENT 1			KIND DATE				APPLICATION NO.							DATE			
ΡI	WO	2007020379			A1		20070222		WO 2006-GB2915						20060804				
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	KR	2008	04289	92		Α	A 2008051				KR 2	-800		20080312					
PRAI	GB	2005	-165	56		Α		2005	0812										
	WO	2006	-GB2	915		W		2006	0804										

OS CASREACT 146:254034; MARPAT 146:254034

AB A continuous carbonylation process for high turnover carbonylation, and a carbonylation reaction medium and product stream thereof. The process comprises carbonylating an ethylenically unsatd. compound with carbon monoxide in the presence of a source of hydroxyl groups and a catalyst system. The catalyst system comprising: (a) a bidentate phosphine, arsine or stibine ligand; and (b) a catalytic metal selected from a group VIB or group VIIIB metal or a compound thereof. The catalytically active concentration of

said catalytic metal, measured as the ACCF (product Kg hr-1 Dm-3), is maintained at less than 0.5.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2005:962129 CAPLUS
- DN 143:250073
- TI Catalyst system for carbonylating ethylenically unsaturated compounds
- IN Eastham, Graham; Tindale, Neil
- PA Lucite International UK Limited, UK

CODEN: PIXXD2 DT Patent LA English FAN.CNT 1 KIND DATE APPLICATION NO. DATE WO 2005079981 A1 001 PATENT NO. A1 20050901 WO 2005-GB569 20050217 \_\_\_\_\_ W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2005215229 A1 20050901 AU 2005-215229 20050217 CA 2005-2555374 EP 2005-717741 CA 2555374 Α1 20050901 20050217 EP 1713582 Α1 20061025 20050217 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS А 20070530 CN 2005-80011699 CN 1972750 20050217 BR 2005-7805 JP 2006-553662 A 20070710 T 20070816 A 20070615 A 20070111 A1 20071206 A 20040218 W 20050217 А BR 2005007805 20070710 20050217 JP 2007522934 20050217 IN 2006-DN4679 IN 2006DN04679 20060814 KR 2007006782 KR 2006-719185 20060918 US 20070282124 PRAI GB 2004-3592 US 2007-589971 20070702 WO 2005-GB569 MARPAT 143:250073 OS The present invention provides a catalyst system capable of catalyzing the AΒ carbonylation of an ethylenically unsatd. compound, which system is obtainable by combining: (A) a metal of Group VIB or Group VIIIB or a compound thereof, (B) a bidentate phosphine, arsine or stibine ligand, and (C) an acid, wherein the ligand is present in at least a 2:1 M excess compared to the metal or the metal in the metal compound, and that the acid is present in at least a 2:1 M excess compared to the ligand, a process for the carbonylation of an ethylenically unsatd. compound, a reaction medium, and use of the system. Thus, Me propanoate was prepared from ethylene, carbonmonoxide and methanol catalyzed by a catalyst system containing tri(dibenzylideneacetone)dipalladium (1.44 x10-5 mol), 1,2-bis-(di-tert-butylphosphinomethyl) ferrocene (7.61 x 1 0-5 mol) and methanesulfonic acid (2.30 x 10-3 mol). THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 3 ALL CITATIONS AVAILABLE IN THE RE FORMAT ANSWER 4 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN L4ΑN 2005:74531 CAPLUS DN142:316919 ΤI Chiral ferrocenyl diphosphines for asymmetric transfer hydrogenation of acetophenone Cabou, Jerome; Brocard, Jacques; Pelinski, Lydie ΑU Laboratoire de Catalyse de Lille, Catalyse Asymetrique et Polymerisation, CS UMR CNRS 8010, ENSCL, Villeneuve d'Ascq, 59 652, Fr. SO Tetrahedron Letters (2005), 46(7), 1185-1188 CODEN: TELEAY; ISSN: 0040-4039 PΒ Elsevier B.V. DT Journal

PCT Int. Appl., 158 pp.

SO

LA

English

- OS CASREACT 142:316919
- AB The synthesis of optically pure ferrocenyl diphosphines have been realized from (R)-(+)-N, N-dimethylaminoethylferrocene. Particularly, dissym. ferrocenyl diphosphines have been synthesized. The diphosphines have been used as ligands in asym. transfer hydrogenation of acetophenone in the presence of Ru catalysts.
- RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:733658 CAPLUS
- DN 142:219391
- TI Ferrocenylmethylphosphines ligands in the palladium-catalysed synthesis of methyl propionate
- AU Butler, Ian R.; Baker, Paul K.; Eastham, Graham R.; Fortune, Kevin M.; Horton, Peter N.; Hursthouse, Michael B.
- CS Department of Chemistry, University of Wales, Gwynedd, LL57 2UW, UK
- SO Inorganic Chemistry Communications (2004), 7(9), 1049-1052 CODEN: ICCOFP; ISSN: 1387-7003
- PB Elsevier B.V.
- DT Journal
- LA English
- OS CASREACT 142:219391
- AΒ The synthesis of a range of novel (ferrocenylmethyl) phosphine ligands is described which have direct application in the palladium-catalyzed reaction of CO, MeOH and ethene to obtain Me propionate, a key intermediate in the preparation of Me methacrylate. Thus, lithiation of CpFeC5H3CH2NMe2 and subsequent quench with Eschenmoser's salt gave 50% 1,2-(Me2NCH2)2C5H3FeCp (1), the structure of which was determined by x-ray crystallog. Refluxing 1 with secondary phosphines HPR2 (R = CMe3, 1-adamantyl; HPR2 = 1,3,5,7-tetramethyl-2,4,8-trioxa-6-phosphaadamantane) in HOAc gave 1,2-(R2PCH2)2C5H3FeCp (3a-c, resp.); 3a was obtained in 83% yield and its structure was determined by x-ray crystallog. Hydroxymethyl analog 1,2-[(HOCH2)2PCH2]2C5H3FeCp (6) was obtained by quaternization of 1 with MeI and subsequent reaction with P(CH2OH)3 and structurally characterized. When these ligands were used in the palladium-catalyzed preparation of Me propionate, typical turnover nos. of 59,000-64,000 were observed
- RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:539457 CAPLUS
- DN 141:350241
- TI The first 1,2,3-tris(phosphinomethyl)ferrocene
- AU Butler, Ian R.; Horton, Peter N.; Fortune, Kevin M.; Morris, Kevin; Greenwell, Christopher H.; Eastham, Graham R.; Hursthouse, Michael B.
- CS Department of Chemistry, University of Wales, Gwynedd, Bangor, LL57 2UW, UK
- SO Inorganic Chemistry Communications (2004), 7(7), 923-928 CODEN: ICCOFP; ISSN: 1387-7003
- PB Elsevier Science B.V.
- DT Journal
- LA English
- OS CASREACT 141:350241
- AB The synthesis of the first 1,2,3-tris(phosphinomethyl)ferrocene is reported using [(dimethylamino)methyl]ferrocenes as useful intermediates. Lithiation of 1,2-bis[(dimethylamino)methyl]ferrocene with subsequent quenching with paraformaldehyde or Eschenmoser's salt afforded 2,3-bis[(dimethylamino)methyl]-1-ferrocenemethanol (9) or 1,2,3-tris[(dimethylamino)methyl]ferrocene (3), resp. Phosphination of 9 by di-tert-butylphosphine in refluxing AcOH gave the title compound,

1,2,3-tris(di-tert-butylphosphinomethyl)ferrocene (8) in 31% yield. Triamine 3 also gave the triphosphine 8 under the same reaction conditions. The crystal structure of 8 is reported.

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
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AN 2004:490809 CAPLUS

DN 141:54780

TI Carbonylation of vinyl acetate and catalyst

IN Eastham, Graham Ronald; Rucklidge, Adam John; Cole-Hamilton, David

PA Lucite International UK Limited, UK

SO PCT Int. Appl., 48 pp. CODEN: PIXXD2

MARPAT 141:54780

DT Patent

LA English

FAN.CNT 4

OS

	PAT	PATENT NO.				KIND DATE			APPLICATION NO.						DATE				
ΡI	WO 2004050599			A1 20040617			WO 2003-GB4679						20031031						
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	AU 2003278375		A1	.1 20040623			AU 2003-278375						20031031						
	EP	IP 1565425 IP 1565425			A1		20050824			EP 2003-769682					20031031				
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	JΡ	2006						2006	0309							2	0031	031	
	ΑT	3867	13			Τ		20080315		AT 2003-769682						20031031			
	ZA	2005	0039.	32		Α		2006	0830	ZA 2005-3932						20050516			
	US	2006	0128	985		A1		2006	0615	US 2005-536801						20051209			
PRAI	GB	2002	-280	18		Α		20021130											
	WO 2003-GB4679 W 20031031																		

AB The title carbonylation of vinyl acetate (I) comprises reacting I with CO in the presence of a source of hydroxyl groups and of a catalyst system, the catalyst system obtained by combining (c) a Group VIIIB metal or a compound, and (d) a bidentate phosphine ligand, to produce a lactate ester or acid of MeCH(OH)C(:O)OR, where R = H, or a C1-30-alkyl or aryl moiety which may be substituted or unsubstituted and either branched or linear or 3-hydroxy propanoate ester or acid of CH2(OH)CH2C(O)OR. In an O free (<10 ppm O2) environment Pd2(dba)3 (0.04 mmoles Pd) and 1,2-bis(di-tertbutylphosphinomethyl)benzene (0.24 mmoles) under N atmospheric, then 300 mL degassed MeOH was added, and the solution was allowed to stir for 1 h, methanesulfonic acid (0.24 mmoles) along with 0.34 g polyvinylpyrollidone dispersant and  $75~\mathrm{mL}$  vinyl acetate (VAM) were added. The reaction mixture was heated to  $85^{\circ}$ , and 10 bar of CO was added causing the temperature to increase to  $100\,^{\circ}$ , where it was held, and the solution allowed to react for 3 h, where both the linear and branched products (methyl-2-acetoxy propanoate and methyl-3-acetoxy propanoate) were produced.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 8 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
L4
ΑN
    2004:252417 CAPLUS
DN
    140:289189
    A catalyst system suitable for carbonylating ethylenically unsaturated
TI
    compounds
ΙN
    Eastham, Graham
PA
    Lucite International Uk Limited, UK
SO
    PCT Int. Appl., 116 pp.
    CODEN: PIXXD2
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                                           IN 2005-DN778
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    ZA 2005001775
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PRAI GB 2002-21093
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                               20021130
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                               20030806
    GB 2002-18613
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    WO 2003-GB3936
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AB The catalyst comprises a Group VIIIB metal or compound thereof and a metallocene. The carbonylation of ethylenically unsatd. compds. using carbon monoxide in the presence of a catalyst system and an alc. or water to yield the corresponding ester or carboxylic acid, resp. An example of the metallocene is 1,2-bis(dimethylaminomethyl)ferrocene.

MARPAT 140:289189

OS

- 2002:565880 CAPLUS ΜA
- 138:39371 DN
- 'User-friendly' primary phosphines and an arsine: synthesis and ΤТ characterization of new air-stable ligands incorporating the ferrocenyl group
- Henderson, William; Alley, Steven R. ΑU
- Department of Chemistry, University of Waikato, Hamilton, 3105, N. Z. CS
- Journal of Organometallic Chemistry (2002), 656(1-2), 120-128 SO CODEN: JORCAI; ISSN: 0022-328X
- РΒ Elsevier Science B.V.
- DT Journal
- LA English
- OS CASREACT 138:39371
- Reaction of FcCH2CH2P(O)(OH)2 or FcCH2P(O)(OH)(OEt) [Fc = AΒ Fe( $\eta$ 5-C5H4)( $\eta$ 5-C5H5)] with excess CH2N2 followed by reduction with Me3SiCl-LiAlH4 gives the air-stable primary phosphines FcCH2CH2PH2 and the previously reported analog FcCH2PH2 in high yields. Reduction of 1,1'-Fc'[CH2P(0)(OEt)2] [Fc' = Fe( $\eta$ 5-C5H4)2] and 1,2-Fc''[CH2P(O)(OEt)2] [Fc'' = Fe( $\eta$ 5-C5H5)( $\eta$ 5-C5H3)] similarly gives the new primary phosphines 1,1'-Fc'(CH2PH2)2 and 1,2-Fc''(CH2PH2)2, resp. The arsine FcCH2CH2AsH2, which is also air-stable, has been prepared by reduction of the arsonic acid FcCH2CH2As(O)(OH)2 using Zn/HCl. An x-ray structure has been carried out on the arsine, which is only the second structure determination of a free primary arsine. The molybdenum carbonyl complex
  - [1,2-Fc''(CH2PH2)2Mo(CO)4] was prepared by reaction of the phosphine with [Mo(CO) 4(pip) 2] (pip = piperidine), and characterized by a preliminary x-ray structure determination However, the same reaction of 1,1'-Fc'(CH2PH2)2 with [Mo(CO) 4(pip) 2] gave [1,1'-Fc'(CH2PH2) 2Mo(CO) 4] and the dimer [1,1'-Fc'(CH2PH2)2Mo(CO)4]2, characterized by electrospray mass spectrometry. 1,1'-Fc'[CH2PH2Mo(CO)5]2 and 1,2-Fc''[CH2PH2Mo(CO)5]2 were likewise prepared from the phosphines and excess [Mo(CO)5(THF)].
- RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4ANSWER 10 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
- ΑN 2000:609611 CAPLUS
- DN 133:281882
- ΤI Diastereoselective 1,2-addition of organometallic reagents to chiral formylferrocenes leading to enantiomerically pure ferrocenyl amino alcohols: application to asymmetric dialkylzinc addition to aldehydes and synthesis of optically active 1,2-homodisubstituted ferrocenes
- ΑU Fukuzawa, Shin-Ichi; Tsuchiya, Daisuke; Sasamoto, Kae; Hirano, Kohki; Ohtaguchi, Makoto
- Department of Chemistry and Applied Chemistry, Institute of Science and CS Engineering, Chuo University, Tokyo, 112-8551, Japan European Journal of Organic Chemistry (2000), (16), 2877-2883
- SO CODEN: EJOCFK; ISSN: 1434-193X
- Wiley-VCH Verlag GmbH PΒ
- DTJournal
- LA English
- CASREACT 133:281882 OS
- AΒ Chiral formylferrocenes were readily prepared in good yields by ortho-lithiation of the TMS-blocked or unblocked aminoferrocenes and subsequent reaction with DMF. The stereochem. of the reaction of 1-[1-(S)-dimethylaminoethyl]-2(Rp)-formylferrocene (I) with organometallic reagents was examined Reactions of I with Grignard and organolithium reagents gave the corresponding amino alc. (II) in good yields with moderate to high diastereomeric excesses (up to 99%). When a dialkylzinc was used as the nucleophile, a single diastereomer was obtained almost exclusively. This reaction may be rationalized in terms of an autocatalytic mechanism; the zinc alkoxide, generated in situ, functions

as an activator of dialkylzinc, which then adds to the formyl group. The asym. diethylzinc addition to benzaldehyde was examined by using formylferrocenes such as I, or ferrocenyl amino alcs. such as II as catalysts, especially with regard to the relationship between catalytic activity

and the chirality of the diastereomeric ferrocenes. Alkylation with I and II gave (1R)-phenyl-1-propanol in good yields with high ee values (87-91% ee). With aromatic, straight-chain, or branched aliphatic aldehydes, the stereoselective alkylation successfully gave the corresponding alcs. in good to high optical purities when I was employed as the catalyst.

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	31.02	209.59
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.00	-8.00

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